

Abstract Submitted
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On the nature of the pressure-induced insulator-to-metal transition

in LaMnO₃ ATSUSHI YAMASAKI, Max-Planck-Institut für Festkörperforschung, MARTIN FELDBACHER, Max-Planck-Institut für Festkörperforschung and Department of Physics and Astronomy, Rutgers University, OLE K. ANDERSEN, KARSTEN HELD, Max-Planck-Institut für Festkörperforschung — Since the discovery of colossal magnetoresistance, manganites have been intensively studied. We focus on the pressure induced insulator-to-metal (IM) transition which was found experimentally [1] in the undoped parent compound LaMnO₃ with configuration $t_{2g}^3 e_g^1$. This transition occurs at room temperature (above $T_N=140$ K) and at a hydrostatic pressure of 32 GPa where the Jahn-Teller distortion appears to be completely suppressed [1]. The IM transition thus seems to be a bandwidth-driven Mott-Hubbard transition of the e_g electrons. We employ the local density approximation combined with static and dynamical mean-field theories (LDA+ U and LDA+DMFT) and conclude that the IM transition observed at 32 GPa in paramagnetic LaMnO₃ at room temperature is *not* a Mott transition, but is caused by the overlap of the majority-spin e_g bands, orbitally polarized by the Coulomb repulsion. Crucial are also the bandwidth reduction of ~ 0.6 and $2/3$ arising from, respectively, the gap generated by the crystal-field splitting and the random, spatially uncorrelated direction of the t_{2g} spin at room temperature. [1] I. Loa *et al.*, Phys. Rev. Lett. **87**, 125501 (2001).

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